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ELASTIC CONSTANTS IN THE ANHARMONIC FERROMAGNETIC CRYSTALS

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1. Introduction

The generalization of the Heisenberg and the Ising models[1], which assume that the spins (magnetic moments) take part in the thermal motions and that the exchange integral depends on the instantaneous positions of the atoms (ions), gives the possibility to investigate correlations between magnetic and mechanical properties of crystals. The usual approach to this problem contains the following assumtpions:

Atomic displacements are small and so the exchange integral can be expanded in powers of the displacements. Restricting ourselves to the first two terms we get, besides the usual Heisenberg (Ising) Hamiltonian, the term linear to the displacement and quadratic in the spin operators which describe spin-phonon interaction.

Lattice dynamics is treated in the harmonic approximation.

A detailed investigation of the various aspects of the spin-phonon interaction in the Heisenberg model under this assumptions is given in[2].

Recently, many works have concerned this approach to the Ising model, especially the interesting problem of the first order phase transitions in some magnetic materials (see for instance [3,4] and the literature there cited). But this approach cannot be applied to certain cases, where anharmonic interaction plays an essential role, e.g., at high temperatures, near lattice structural phase transition pionts, etc. In these cases the anharmonic interaction should be taken into account explicitly.

In order to be able to treat such cases a new method for the investigation of spin-phonon interaction in the Heisenberg model has been proposed in /5,7/. As compared to the conventional approach /2/, this method is not restricted only to consideration of the linear terms in the expansion of the exchange integral and allows one to consider in self-consistent manner the effects of the anharmonicity in lattice vibrations.

We also mention here the work /8/, which gives some arguments that the first order phase transition might occur in a compressible anharmonic lattice though the corresponding harmonic lattice does not undergo a first order transition.

In this respect it is interesting to calculate some of quantities, which have anomalous behaviour near a magnetic phase transition (elastic constants, thermal expansivity, etc.), considering Heisenberg or Ising Model on a compressible lattice allowing for arbitrary anharmonicities of the bare lattice.

The purpose of this paper is to present an approximate, microscopic calculation of the isothermal elastic constants of the anharmonic ferromagnetic crystals, using the self-consistent spin-phonon interaction theory /5-7/. Some earlier calculations of the ferromagnetic elastic constants /3,9/ did not take into account the anharmonicities of lattice vibrations.

For the experimental results we refer the reader to the review /10/.

Elastic constants of pure lattice can be calculated by the method of homogeneous deformation and by that of long waves /11/. The results obtained by using both methods are consistent in the cases of harmonic /11/ and anharmonic /12/ lattices.

We shall calculate isothermal elastic constants using the method of long waves and the fact that three independent elastic constants of the cubic lattices can be found from the dispersion curve inclination

In Section 2 we give the calculation of the phonon frequencies taking into account spin-phonon interactions of all orders. In Section 3 high-temperature isothermal elastic constants of f.c.c. lattice are given. At the end of this section we consider approximately the influence of spin system on the elastic constants.

2. The Hamiltonian and the Phonon Green Function

We consider a magnetic anharmonic crystal which can be described by the Hamiltonian /7/:

$$H = -(2M)^{-1}\sum_{\ell} \vec{\nabla}_{\ell}^{2} + U(\vec{R}_{\ell}) - \frac{1}{2}\sum_{\ell m} J(\vec{R}_{\ell} - \vec{R}_{m})\vec{S}_{\ell}\vec{S}_{m}, \quad (1)$$

where $\vec{R}_\ell$ and $\vec{S}_\ell$ are the position and the spin of the atom with mass M in the lattice site $\vec{x}_\ell = \langle\vec{R}_\ell\rangle$; the thermal average $\langle\ldots\rangle$ is taken with Hamiltonian (1). Using an expansion of the potential energy of crystal $U(\vec{R}_\ell)$ and of the exchange energy $J(\vec{R}_\ell - \vec{R}_m)$ in the infinite series in thermal displacement $\vec{u}_\ell = \vec{R}_\ell - \vec{x}_\ell$ we get the equation of motion for the Fourier transform of the retarded phonon Green function $G_{ii'}(t-t') = \langle\langle u_i(t); u_{i'}(t')\rangle\rangle$, $(i = \ell, \alpha)$ in the form /5-7/:

$$G_{ii'}(\omega) = G^{\circ}_{ii'}(\omega) + \sum_{n=2}^{\infty}\frac{1}{n!}\sum_{j1\ldots n} G^{\circ}_{ij}(\omega)\,\Phi_{j1\ldots n}\langle\langle u_1\ldots u_n | u_{i'}\rangle\rangle^{ir}_{\omega} -$$

$$-\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{j\ell m1\ldots n} G^{\circ}_{ij}(\omega)\langle\langle u_1\ldots u_n \vec{S}_\ell\vec{S}_m | u_{i'}\rangle\rangle^{ir}_{\omega}\,\nabla_j\nabla_1\ldots\nabla_n \times \quad (2)$$

$$\times\frac{1}{2}\langle J(\vec{R}_\ell - \vec{R}_m)\rangle,$$

where we have introduced irreducible (ir) Green function /6,7/:

$$\langle\langle\{u_1(t)\ldots u_n(t)\vec{S}_\ell(t)\cdot\vec{S}_{\ell'}(t)\}; u_{i'}(t)\rangle\rangle^{ir} = \langle\langle\{u_1\ldots u_n(\vec{S}_\ell\vec{S}_{\ell'}) -$$

$$-\langle u_1\ldots u_n(\vec{S}_\ell\vec{S}_{\ell'})\rangle\}; u_{i'}\rangle\rangle -$$

$$-\sum_{m=0}^{n-1} C_n^m \langle u_{m+1}\ldots u_n\rangle\langle\langle\{u_1\ldots u_m(\vec{S}_\ell\vec{S}_{\ell'})\}; u_{i'}\rangle\rangle^{ir} -$$

$$-\sum_{m=1}^{n} C_n^m < u_{m+1} \dots u_n (\vec{S}_\ell \; \vec{S}_{\ell'} \;) >\ll \{ u_1 \dots u_m \}; u_{i'} \gg^{ir} \tag{2a}$$

$$C_n^m = n! / m! (n-m)!$$

which cannot be simplified by the decoupling of the equal time operators and the effective phonon-phonon interaction:

$$\tilde{\Phi}_{1\dots n} = \nabla_1 \dots \nabla_n \{ < U(\vec{R}_\ell) > - \frac{1}{2} \sum_{\ell m} < J(\vec{R}_\ell - \vec{R}_m) \vec{S}_\ell \vec{S}_m > \cdot \tag{3}$$

The zero-order Green function $G^{\circ}_{ii'}(\omega)$ is defined by the equation

$$\sum_j (M\omega^2 \delta_{ij} - \tilde{\Phi}_{ij}) G^{\circ}_{ji'}(\omega) = \delta_{ii'} \tag{4}$$

and it describes the propagation of the undamped self-consistent phonons /5,6/. In order to obtain the damping of the phonons it is necessary to consider the equation of motion for the irreducible Green function $\ll A(t); u_{i'}(t')\gg$ in (2) by differentiating it with respect to time argument t'. As a result we can rewrite the equation (2) in the matrix form $G = G^{\circ} + G^{\circ} P G^{\circ}$, where $P_{jj'}(\omega)$ is equal to the sum of products composed of the Green functions $\ll A|B \gg^{ir}$ $(A, B = \{u_1 \dots u_r\}$ or $\{u_1 \dots u_n (\vec{S}_\ell \vec{S}_m)\})$ and two corresponding vertex functions of the phonon-phonon and spin-phonon interactions.

Now introducing the phonon self-energy operator Π according to the equation $G = G^{\circ} + G^{\circ} \Pi G$ we get /7/:

$$\Pi_{ii'}(\omega + i\epsilon) = \{ P (1 + G^{\circ} P)^{-1} \} = \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega' + i\epsilon} (e^{\omega'/\theta} - 1) \times$$

$$\times \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{-i\omega' t} \{ \sum_{n=1}^{\infty} \frac{1}{n!} (\sum_{jj'} < u_j(t) u_{j'} > \nabla_j \nabla_{j'})^n \times$$

$$\times \tilde{\Phi}_i (\dots \vec{x}_i \dots) \tilde{\Phi}_{i'} (\dots \vec{x}_{i'} \dots) +$$

$$+e^{(\sum_{jj'}\langle u_j(t)u_{j'}\rangle \nabla_j \nabla_{j'})} \frac{1}{4}\sum_{\ell m\ell' m'} \langle (\vec{S}_\ell(t)\vec{S}_m(t))(\vec{S}_{\ell'}\vec{S}_{m'})\rangle^{ir} \times$$

$$\times \nabla_i \langle J(\vec{R}_\ell - \vec{R}_m)\rangle \nabla_{i'} \langle J(\vec{R}_{\ell'} - \vec{R}_{m'})\rangle, \qquad (5)$$

where the approximate explicit form is obtained in the second order in spin-phonon and phonon-phonon (3) interaction by using the spectral representation for the retarded Green function $\langle\langle A|B\rangle\rangle^{ir}_\omega$ in terms of the two time correlation functions. According to the definition (2a) the irreducible four-spin correlation function in (5) is given by the expression:

$$\langle(\vec{S}_\ell(t)\vec{S}_m(t))(\vec{S}_{\ell'}\vec{S}_{m'})\rangle = \langle(\vec{S}_\ell(t)\vec{S}_m(t) - \langle\vec{S}_\ell\vec{S}_m\rangle)(\vec{S}_{\ell'}\vec{S}_{m'} -$$

$$-\langle\vec{S}_{\ell'}\vec{S}_{m'}\rangle)\rangle \qquad (5a)$$

The inelastic phonon-phonon interaction in all orders (the first term in (5)) and the inelastic spin-phonon interaction (the four-spin two-time correlation function) with additional excitation of phonons $(\exp\{\ldots\})$ in the second term in (5) are explicitly taken into account in the phonon self-energy operator (5).

After the Fourier transformation of the Green function of the displacement operators

$$\langle\langle u^\alpha_\ell | u^\beta_{\ell'}\rangle\rangle_\omega = \frac{1}{MN}\sum_{\vec{q}j} \frac{e^\alpha_{\vec{q}j}\, e^\beta_{\vec{q}j}}{2\omega_{\vec{q}j}} e^{i\vec{q}(\vec{\ell}-\vec{\ell}')} G_{\vec{q}j}(\omega), \qquad (6)$$

we get following expression for the Green functions $G_{\vec{q}j}(\omega)$[14]:

$$G_q(\omega) = \frac{2\omega_q}{\omega^2 - \omega_q^2 - 2\omega_q \Pi_q(\omega)}. \qquad (7)$$

Further we shall investigate only the case of f.c.c. lattice, We take the nearest neighbour central force interactions for lattice interactions

$$U = \frac{1}{2} \sum_{\ell \neq m}{}' \phi\left(|\vec{R}_\ell - \vec{R}_m|\right), \qquad (8)$$

where prime on the summation means that the second summation is performed only over z nearest neighbours (for f.c.c. lattice $z = 12$). The spin system will be investigated in the nearest neighbour approximation too.

Using the upper assumptions and the equation (4), the frequencies $\omega_q \{q=(\vec{q},j)\}$ in equation (3) can be determined in the pseudo-harmonic approximation /14/ by the equation

$$\omega^2_{\vec{q}j} = \frac{\tilde{f}(\theta,\ell)}{M} \sum_{\ell} \frac{(\vec{\ell}, \vec{e}_{\vec{q}j})^2}{\ell^2} (1 - e^{i\vec{q}\vec{\ell}}) = \frac{\tilde{f}(\theta,\ell)}{f} \omega^2_{0\vec{q}j} . \qquad (9)$$

Taking into account only the nearest neigbour interactions the pseudoharmonic renormalization is reduced to that of strength constant $\tilde{f}(\theta, \ell)$, where $\omega_{0\vec{q}j}$ is the harmonic frequency corresponding to the strength constant f.

The Fourier transformation of the self-energy operator (5), taking into account only the renormalized cubic anharmonicity ($n=2$ in the first term of eq. (5)) and neglecting the additional excitations of phonons ($\exp(\ldots) \approx 1$) in the second term in (5), gives

$$\Pi_q(\omega) = \sum_{q_1 q_2} |\tilde{\tilde{\Phi}}_3(-q, q_1, q_2)|^2 \left\{ \frac{(\omega_{q_1} + \omega_{q_2})[1 + n(\omega_{q_1}) + n(\omega_{q_2})]}{\omega^2 - (\omega_{q_1} + \omega_{q_2})^2} - \right.$$

$$\left. - \frac{(\omega_{q_1} - \omega_{q_2})[n(\omega_{q_1}) + n(\omega_{q_2})]}{\omega^2 - (\omega_{q_1} - \omega_{q_2})^2} \right\} + \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega' + i\epsilon} (e^{\omega'/\theta} - 1) C_q(\omega),$$

where (10)

n) $n(\omega) = (e^{\omega/\theta} - 1)^{-1}$

$$\tilde{\tilde{\Phi}}_3(q_1, q_2, q_3) = \frac{\Delta(\vec{q}_1 + \vec{q}_2 + \vec{q}_3)}{(2N)^{3/2}} \sum_{\substack{\vec{s}_1 \vec{s}_2 \vec{s}_3 \\ a_1 a_2 a_3}} \tilde{\tilde{\Phi}}^{a_1 a_2 a_3}_{s_1 s_2 s_3} \times \tag{11}$$

$$\times \Pi \left(\frac{e^{a_i}_{q_i}}{\sqrt{M\omega_{q_i}}} e^{i \vec{q}_i \vec{s}_i} \right)$$

$$C_q(\omega) = \frac{N[\tilde{J}'(\ell)]^2}{2} \sum_{\vec{q}_1 \vec{q}_2} \frac{(\vec{\ell}, \vec{e}_{qj})(\vec{\ell}', \vec{e}_{qj})}{M\omega_{\vec{q}j} \; |\vec{\ell}||\vec{\ell}'|} \sin \frac{1}{2}(\vec{q}\,\vec{\ell}) \sin \frac{1}{2}(\vec{q}\,\vec{\ell}') \times$$

$$\times e^{-i\frac{1}{2}\vec{q}\vec{\ell}} \, e^{i\frac{1}{2}\vec{q}\vec{\ell}'} \, e^{i(\vec{q}-\vec{q}_1)\vec{\ell}} \, e^{-i(\vec{q}+\vec{q}_2)\vec{\ell}'} \times \tag{12}$$

$$\times \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{-i\omega t} \langle (\vec{S}_{\vec{q}_1}(t) \vec{S}_{\vec{q}-\vec{q}_1}(t)) (\vec{S}_{\vec{q}_2} \vec{S}_{-\vec{q}-\vec{q}_2}) \rangle^{ir}.$$

The four-spin Fourier transformed correlation function in (12) is obtained by means of representation

$$\vec{S}_\ell = \sum_{\vec{q}} e^{i\vec{q}\vec{x}_\ell} \vec{S}_{\vec{q}} .$$

For the central pair force model we can calculate $|\tilde{\tilde{\Phi}}_3|^2$ analogously with [14] and get:

$$|\tilde{\tilde{\Phi}}_3(-q, q_1, q_2)|^2 = \frac{\Delta(\vec{q}_1 + \vec{q}_2 - \vec{q})}{4M^3 N\omega_q \omega_{q_1} \omega_{q_2}} \tilde{g}^2(\theta, \ell) F^2(-q, q_1, q_2) \tag{13}$$

where

$$F(\vec{q}j, \vec{q}_1 j_1, \vec{q}_2 j_2) = \sum_n{}' (-1)^{\frac{d}{2}\vec{r}\vec{n}} (\vec{n}, \vec{e}_{\vec{q}j})(\vec{n}, \vec{e}_{\vec{q}_1 j_1})(\vec{n}, \vec{e}_{\vec{q}_2 j_2}) \times$$

$$\times \sin \frac{d}{4}(\vec{n}\vec{q}) \sin \frac{d}{4}(\vec{n}\vec{q}_1) \sin \frac{d}{4}(\vec{n}\vec{q}_2) \tag{14}$$

is dimensionless sum over the lattice points, $n = \ell|(\frac{d}{2})$, d is lattice constant, ℓ is the distance between the nearest neighbours, $2\pi\tau$ is the reciprocal lattice vector.

The strength constants $\tilde{f}(\theta,\ell)$ and $\tilde{g}(\theta,\ell)$ in the equations (9) and (13) are determined in the self-constant manner:

$$\tilde{f}(\theta,\ell)=\tilde{\phi}''(\ell)-\tilde{J}''(\ell)\langle\vec{S}_\ell\vec{S}_0\rangle,\ \tilde{g}(\theta,\ell)=\tilde{\phi}'''(\ell)-\tilde{J}'''(\ell)\langle\vec{S}_\ell\vec{S}_0\rangle, \quad (15)$$

where $\tilde{\phi}(\ell)$ and $\tilde{J}(\ell)$ are self-consistent potential energy and exchange integral respectively. In the pseudoharmonic approximation these quantities take the form /14/:

$$\tilde{\phi}(\ell)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{1}{2}\overline{u^2}\right)^n\phi^{(2n)}(\ell),$$

$$\tilde{J}(\ell)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{1}{2}\overline{u^2}\right)^n J^{(2n)}(\ell). \quad (16)$$

The mean square relative displacement of neighbouring atoms $\overline{u^2}(\ell)$ can be expressed using the Green functions (6) and (7) as

$$\overline{u^2}(\ell)=\frac{\langle[\vec{\ell}(u_\ell-u_0)]^2\rangle}{\ell^2}=\frac{1}{z\tilde{f}(\theta,\ell)}\sum_k\omega_k\frac{1}{\pi}\int_{-\infty}^{+\infty}d\omega\coth\frac{\omega}{2\theta}\times \quad (17)$$
$$\times\ [-\mathrm{Im}G_k(\omega+i\epsilon)].$$

It should be noted, that in strength constants (15), besides the pseudoharmonic renormalization /14/, spin-phonon interaction gives the new term proportional to the spin pair correlation function $\langle\vec{S}_\ell\vec{S}_0\rangle$.

The equilibrium lattice constant $d=\ell\sqrt{2}$ is obtained from the equation of state for ferromagnetic anharmonic crystals /6/, which in our case takes the form

$$P=-\frac{z\ell}{6v}\left(\tilde{\phi}'(\ell)-\langle\vec{S}_\ell\vec{S}_0\rangle\tilde{J}'(\ell)\right), \quad (18)$$

where $v=V/N=\ell^3\sqrt{2}$ and P is the external pressure. Thus the self-consistent system of equations (16), (17) and (18) gives us the equilibrium parameters of the lattice, the renormalized phonon frequencies $\tilde{\omega}_{\vec{q}j}$ and phonon widths $\Gamma_{\vec{q}j}$:

$$\tilde{\omega}_{\vec{q}j} = \omega_{\vec{q}j} + \mathrm{Re}\,\Pi_{\vec{q}j}(\omega_{j}),\ \Gamma_{qj}(\omega) = -\mathrm{Im}\,\Pi_{\vec{q}j}(\omega + i\epsilon). \qquad (19)$$

3. Elastic Constants for f.c.c. Lattice

Further we shall investigate only the case of a classical high temperature region: $\theta = kT \gg \theta_D$ and $\theta \gg E_{max}(\theta)$, where θ_D is Debye temperature and $E_{max}(\theta)$ is a maximum energy of spin excitations at temperature θ, when an expression $(e^{\omega'/\theta} - 1) \approx \frac{\omega'}{\theta}$ is possible in (10). We put also $\theta_C > \theta_D$. On the basis of these assumptions the self-energy operator (10) takes the form:

$$\Pi_{\vec{q}j}(\omega) \simeq -\theta\,\omega_{\vec{q}j}\,\frac{\tilde{g}^2(\theta,\ell)}{\tilde{f}^3(\theta,\ell)}S_{\vec{q}j}(\omega) + \frac{1}{\theta}\int_{-\infty}^{+\infty}\frac{\omega' C(\omega')d\omega'}{\omega - \omega' + i\epsilon}, \qquad (20)$$

where

$$S_{\vec{q}j}(\nu) = \frac{1}{32N}\sum_{q_1 q_2}\frac{\Delta(\vec{q}_1 + \vec{q}_2 - \vec{q})}{\lambda^2_{q_1}\lambda^2_{q_2}\lambda^2_{q}}F^2(-q, q_1, q_2)\times$$

$$\times\left\{\frac{(\lambda_{q_1} + \lambda_{q_2})^2}{(\lambda_{q_1} + \lambda_{q_2})^2 - \nu^2} + \frac{(\lambda_{q_1} - \lambda_{q_2})^2}{(\lambda_{q_1} - \lambda_{q_2})^2 - \nu^2}\right\} \qquad (21)$$

$$\nu = \frac{2\omega}{\omega_L};\ \lambda_q \equiv \lambda_{qj} = 2\omega_{\vec{q}j}/\omega_L;\quad \omega_L = \frac{8\tilde{f}(\theta\ell)}{M}.$$

The first term of the self-energy operator (10) differs from the corresponding expression in the absence of a spin-phonon interaction in [14] by the renormalization of strength constants and has been obtained in an analogous way. The second term in (20), proportional to the spin-phonon interaction constant $[\tilde{J}'(\ell)]^2$ and four-spin correlation function $\langle(\vec{S}_{\vec{q}_1}\vec{S}_{\vec{q}-\vec{q}_1})(\vec{S}_{\vec{q}_2}\vec{S}_{\vec{q}-\vec{q}_2})\rangle_\omega^{ir}$ describes the effect of inelastic scattering of phonons by spin excitations.

Three independent isothermal elastic constants of f.c.c. lattice can be found from the dispersion curves inclination /13/. In the static ($\omega=0$) long-wave limit ($\vec{q}\to 0$), with the definite choice of the wave vector $\vec{k}=\vec{q}/q$ along one of summetric crystal directions and polarization $j=L$ (longitudinal) or $j=T_1,T_2$ (one of transversal), one can get the following expressions for isothermal elastic constants /13,15/:

$$\begin{aligned}
&\vec{k}=[1,0,0]\quad \rho\tilde{\omega}^2_{\vec{q},L}\to c_{11}q^2,\quad \rho\tilde{\omega}^2_{\vec{q},T}\to c_{44}q^2,\\
&\vec{k}=[1,1,0)]\quad \rho\tilde{\omega}^2_{\vec{q},T_1}\to c_{44}q^2,\ \rho\tilde{\omega}^2_{\vec{q},T_2}\to\frac{1}{2}(c_{11}-c_{12})q^2,
\end{aligned}\qquad (22)$$

where $\rho=\frac{M}{V}$.

So the calculations of static, long-wave limit of phonon frequencies(19) with the self-energy (20) gives the isothermal elastic constants of anharmonic ferromagnetic crystal:

$$\begin{aligned}
\frac{C_{\alpha\beta}}{C^{(0)}_{\alpha\beta}}=&\frac{R_0}{\ell}\,\frac{\tilde{f}(\theta,\ell)}{f}\Big[1-2\theta\,\frac{\tilde{g}^2(\theta,\ell)}{\tilde{f}^3(\theta,\ell)}S_{\vec{k}j}\Big]-\\
&-\frac{[\tilde{J}'(\ell)]^2N}{4\theta v C^{(0)}_{\alpha\beta}}\sum_{\ell\ell'\vec{q}_1\vec{q}_2}\frac{(\vec{\ell},\vec{e}_{\vec{q}j})(\vec{\ell}',\vec{e}_{\vec{q}j})}{|\vec{\ell}|\,|\vec{\ell}'|}(\vec{k},\vec{\ell})(\vec{k},\vec{\ell}')\times\\
&\times\cos(\vec{q}_1\vec{\ell})\cos(\vec{q}_1\vec{\ell})\langle(\vec{S}_{\vec{q}_1}\vec{S}_{-\vec{q}_1})(\vec{S}_{\vec{q}_2}\vec{S}_{-\vec{q}_2})\rangle,
\end{aligned}\qquad (23)$$

where R_0 is equilibrium distance between the nearest atoms in the harmonic approximation, $C^{(0)}_{\alpha\beta}$ are isothermal elastic constants of harmonic lattice, $S_{\vec{k}j}=\lim_{\vec{q}\to 0}S_{\vec{q}j}$ ($\omega=0$).

The first and the second terms in eq. (23) give the renormalized lattice elastic constants of /15/. The third term in (23), proportional to four-spin correlation function and spin-phonon interaction constant, appears as a consequence of spin-phonon interaction.

Further we shall give an approximate investigation of the third term in (23) in order to get some more information about its influence on the elastic constants.

In the paramagnetic region ($\theta > \theta_c$) in the absence of any external magnetic fields, the quantity $\langle S_i^{\alpha}(t) \rangle$ is equal to zero and we therefore approximate the four-spin correlation function by a sum of products of all possible pair correlations [16]:

$$\langle (\vec{S}_{\vec{q}_1} \vec{S}_{-\vec{q}_1})(\vec{S}_{\vec{q}_2} \vec{S}_{-\vec{q}_2}) \rangle^{ir} = \sum_{\alpha\beta} \langle (S^{\alpha}_{\vec{q}_1} S^{\alpha}_{-\vec{q}_1})(S^{\beta}_{\vec{q}_2} S^{\beta}_{-\vec{q}_2}) \rangle^{ir} \simeq$$

$$\simeq \sum_{\alpha} |\langle S^{\alpha}_{\vec{q}_1} S^{\alpha}_{-\vec{q}_1} \rangle|^2 \{ \delta_{\vec{q}_1, -\vec{q}_2} + \delta_{\vec{q}_1, \vec{q}_2} \}. \qquad (24)$$

Spin-pair correlation functions in (24) can be calculated by the method of work [17], for instance. In the paramagnetic region the rotational invariance condition is fulfilled [17]:

$$\langle S^{x}_{\vec{q}_1} S^{x}_{-\vec{q}_1} \rangle = \langle S^{y}_{\vec{q}_1} S^{y}_{-\vec{q}_1} \rangle = \langle S^{z}_{\vec{q}_1} S^{z}_{-\vec{q}_1} \rangle = \frac{\theta}{N} \frac{\chi}{1 + 2\chi (J_0 - J_{\vec{q}_1})}, \qquad (25)$$

where susceptibility $\chi = \lim_{h \to 0} \sigma / h$ has to be determined from the equation

$$\frac{1}{2\chi} = \frac{\theta}{N} \sum_{\vec{q}} \frac{2}{1 + 2\chi (J_0 - J_{\vec{q}})}. \qquad (26)$$

Susceptibility given by eq. (26) is proportional to $1/\theta^2$ when $\theta \to \infty$ and in the right vicinity of Curie temperature $\chi \sim (\theta - \theta_c)^{-2}$. Substituting (25) into (23) an additional term of the renormalized lattice elastic constants (third term in (23)), which we denote by $C^{(s)}_{\alpha\beta} / C^{(0)}_{\alpha\beta}$, takes the form:

$$\frac{C^{(s)}_{\alpha\beta}}{C^{(0)}_{\alpha\beta}} = - \frac{3\theta [\vec{J}(\ell)]^2}{v C^{(0)}_{\alpha\beta}} \sum_{\ell \ell' j} \frac{(\vec{\ell}, \vec{e}_{\vec{q}j})(\vec{\ell}', \vec{e}_{\vec{q}j})}{|\vec{\ell}||\vec{\ell}'|} (\vec{k}, \vec{\ell})(\vec{k}, \vec{\ell}') \times$$

$$\times \frac{1}{N} \sum_{\vec{q}_1} \frac{\chi^2 \cos(\vec{q}_1 \vec{\ell}) \cos(\vec{q}_1 \vec{\ell}')}{[1 + 2\chi(\tilde{J}_0 - J_{\vec{q}_1})]} . \tag{27}$$

We replace discrete summation over the first Brillouin zone by an integral over Debye zone in (27):

$$\lim_{N\to\infty} \frac{1}{N} \sum_{\vec{q}} (\ldots) \to \frac{v}{(2\pi)^3} \int_0^{q_0} q^2 dq \int_0^{2\pi} d\phi \int_{-1}^{1} d\mu (\ldots), \tag{28}$$

where $\mu = \cos\theta$ and $q_0 = (6\pi^2/v)^{1/3}$. The dominant contribution to the integral in the (27) comes from the region of small q_l and thus for convenience in performing the angular integration over μ we approximate $\cos(\vec{q}_1 \vec{\ell}) \cos(\vec{q}_1' \vec{\ell}') \simeq 1$. After the integration in the equation (27) we get:

$$\frac{C^{(s)}_{\alpha\beta}}{C^{(0)}_{\alpha\beta}} = -\theta \frac{3[\tilde{J}'(\ell)]^2 \chi^{1/2}}{8\pi^2 (2d\, \tilde{J}(\ell))^{3/2} C^{(0)}_{\alpha\beta}} \Big[\sum_{\ell} \frac{(\vec{\ell}, \vec{e}_{\vec{q}j})(\vec{k}, \vec{\ell})}{|\vec{\ell}|} \Big]^2 \times \tag{29}$$

$$\times \Big\{ \operatorname{arctg} q_0 d \sqrt{2\chi \tilde{J}(\ell)} - \frac{q_0 d \sqrt{2\chi \tilde{J}(\ell)}}{1 + 2\chi q_0^2 d^2 \tilde{J}(\ell)} \Big\} .$$

The change of the elastic constants by the spin-phonon interaction, given by (29), agrees qualitatively with experiment /10/. This expression shows that the additional term to the elastic constants increases in absolute value when the temperature approaches to the Curie temperature and has negative sign. Factorization (24) is invalid when $\theta = \theta_c$ and in the vicinity of Curie temperature /16/, so we cannot give the estimation of (29) in these cases. When $\theta \to \infty$ $C^{(s)}_{\alpha\beta} / C^{(0)}_{\alpha\beta} \to 0$.

In conclusion we would like to point out that the main advantage of our approach, as compared to usual approach

([2] and [6] for instance), consists in taking into account in a self consistent manner the anharmonicity of lattice vibrations and higher order terms of spin-phonon interaction.

The aim of the present work was to show how one can calculate isothermal elastic constants of anharmonic ferromagnetic crystals, and further approximations for the four-spin correlation function serve only for qualitative check of calculations. The approximate solution (23), which contain four-spin correlation function, gives the possibility, when a better theory for the Heisenberg model will be develcped, to obtain more reliable quantitative estimations which can be used for comparison with experiment. In our approach it is also necessary to choose the models for lattice potential and exchange integral and to find numerical solutions of self-consistent system of equations (16), (17) and (18) for the equilibrium lattice parameters.

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